Glutaric acid, 2-methylpent-3-yl 2-isopropoxyphenyl ester

Inchi: InChI=1S/C20H30O5/c1-6-16(14(2)3)24-19(21)12-9-13-20(22)25-18-11-8-7-10-17(18)23

InchiKey: CDILUCRMTVWCAR-UHFFFAOYSA-N

Formula: C20H30O5

SMILES: CCC(OC(=O)CCCC(=O)Oc1ccccc1OC(C)C)C(C)C

Mol. weight [g/mol]: 350.45

Physical Properties

Property code	Value	Unit	Source
gf	-359.86	kJ/mol	Joback Method
hf	-868.73	kJ/mol	Joback Method
hfus	37.40	kJ/mol	Joback Method
hvap	82.61	kJ/mol	Joback Method
log10ws	-5.35		Crippen Method
logp	4.527		Crippen Method
mcvol	289.650	ml/mol	McGowan Method
pc	1348.67	kPa	Joback Method
rinpol	2303.00		NIST Webbook
rinpol	2303.00		NIST Webbook
tb	862.34	K	Joback Method
tc	1068.67	K	Joback Method
tf	475.65	K	Joback Method
vc	1.095	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	908.63	J/mol×K	862.34	Joback Method
cpg	924.59	J/mol×K	896.73	Joback Method
cpg	939.25	J/mol×K	931.12	Joback Method
cpg	952.62	J/mol×K	965.51	Joback Method
cpg	964.70	J/mol×K	999.90	Joback Method
cpg	975.51	J/mol×K	1034.28	Joback Method
cpg	985.06	J/mol×K	1068.67	Joback Method
dvisc	0.0006133	Pa×s	475.65	Joback Method

dvisc	0.0002784	Pa×s	540.10	Joback Method
dvisc	0.0001496	Pa×s	604.55	Joback Method
dvisc	0.0000906	Pa×s	668.99	Joback Method
dvisc	0.0000599	Pa×s	733.44	Joback Method
dvisc	0.0000424	Pa×s	797.89	Joback Method
dvisc	0.0000315	Pa×s	862.34	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391868&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume